

SAFETY DATA SHEET

Version 8.2
Revision Date 07/28/2021
Print Date 07/29/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2,6-Dimethyl-4-heptanone

Product Number : 537691
Brand : Aldrich**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +1 314 771-5765
Fax : +1 800 325-5052**1.4 Emergency telephone**Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-
527-3887 CHEMTREC (International) 24
Hours/day; 7 Days/week**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226

Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal word

Warning

Hazard statement(s)

H226

Flammable liquid and vapor.

H335

May cause respiratory irritation.

Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P403 + P235	Store in a well-ventilated place. Keep cool.
P405	Store locked up.
P501	Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : Diisobutyl ketone
Isovalerone
DIBK

Component	Classification	Concentration
2,6-Dimethylheptan-4-one		
CAS-No. 108-83-8 EC-No. 203-620-1 Index-No. 606-005-00-X	Flam. Liq. 3; STOT SE 3; H226, H335 Concentration limits: >= 10 %: STOT SE 3, H335;	>= 50 - < 70 %
3,3,5-trimethylcyclohexanone		
CAS-No. 873-94-9 EC-No. 212-855-9	Flam. Liq. 4; Eye Irrit. 2A; STOT SE 3; H227, H319, H335	>= 5 - < 10 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower.

In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemisorb®). Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Change contaminated clothing. Wash hands after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
2,6-Dimethylheptan-4-one	108-83-8	TWA	25 ppm	USA. ACGIH Threshold Limit Values (TLV)
		TWA	25 ppm 150 mg/m ³	USA. NIOSH Recommended Exposure Limits
		TWA	50 ppm 290 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	25 ppm 150 mg/m ³	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	25 ppm 150 mg/m ³	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

8.2 Exposure controls

Appropriate engineering controls

Change contaminated clothing. Wash hands after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 60 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	165 - 170 °C 329 - 338 °F - lit.
g) Flash point	49 °C (120 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	0.808 g/mL at 25 °C (77 °F) - lit.
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

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10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

Strong bases, Strong oxidizing agents, Strong acids, Strong reducing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages: , damage of respiratory tract

Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Mixture may cause respiratory irritation.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Hazardous properties cannot be excluded but are unlikely when the product is handled appropriately.

Stomach - Irregularities - Based on Human Evidence

Components

2,6-Dimethylheptan-4-one

Acute toxicity

LD50 Oral - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - 4 h - > 14.5 mg/l

(OECD Test Guideline 403)

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: Does not cause skin sensitization.

(OECD Test Guideline 406)

Germ cell mutagenicity

No data available

Test Type: Ames test

Test system: *S. typhimurium*

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

3,3,5-trimethylcyclohexanone

Acute toxicity

LD50 Oral - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 401)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

LC50 Inhalation - Rat - male - 4 h - 14.2 mg/l

(OECD Test Guideline 403)

Symptoms: Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract

Inhalation: absorption

LD50 Dermal - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation

(OECD Test Guideline 404)

Serious eye damage/eye irritation

No data available

Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation.

Acute oral toxicity - Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Acute inhalation toxicity - Shortness of breath, Cough, mucosal irritations, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

SECTION 12: Ecological information

12.1 Toxicity

Mixture

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

No data available

Components

2,6-Dimethylheptan-4-one

Toxicity to fish	flow-through test LC50 - Oncorhynchus mykiss (rainbow trout) - 30 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	Immobilization EC50 - Daphnia magna (Water flea) - 37.2 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	Growth inhibition EC50 - Pseudokirchneriella subcapitata (green algae) - 46.9 mg/l - 72 h (OECD Test Guideline 201)

3,3,5-trimethylcyclohexanone

Toxicity to fish	static test LC50 - Danio rerio (zebra fish) - > 100 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 180 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 82.27 mg/l - 72 h (OECD Test Guideline 201)
	static test NOEC - Desmodesmus subspicatus (green algae) - > 82.27 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - activated sludge - 755 mg/l - 3 h (OECD Test Guideline 209)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1157 Class: 3 Packing group: III
Proper shipping name: Diisobutyl ketone
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1157 Class: 3 Packing group: III EMS-No: F-E, S-D
Proper shipping name: DIISOBUTYL KETONE

IATA

UN number: 1157 Class: 3 Packing group: III
Proper shipping name: Diisobutyl ketone

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information

Further information

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See

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